

# Direct-effect radiation damage in sugars: a combined EMR and DFT study

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The harmful effects of high-energy radiation to organic matter, like cancer, are well known. While insight in the radiation-induced biochemical processes is rapidly evolving, a mechanistic understanding of the initial stages of the radiation physics/chemistry, especially for the *direct* radiation effect, is still lacking. The complexity of macromolecules like DNA and proteins thwarts detailed analysis of the radiation defects in these systems, so that simpler and better controllable model systems need to be used. In this context, we study radicals induced by X-rays in organic molecular solids of sugars, sugar phosphates and amino acids, using a combination of electron magnetic resonance (EMR) experiments and molecular modeling based on density functional theory (DFT). Our results are also of value for dosimetric purposes since the intensity of the electron paramagnetic resonance (EPR) spectrum is an excellent indicator of the radiation dose. An overview of our results within this research theme over the past few years will be presented.

Radical structures are identified by comparing *g* and hyperfine tensors, determined via EMR experiments (EPR and electron-nuclear double resonance (ENDOR)) on single crystals, with theoretical values obtained from state-of-the-art DFT simulations using periodic boundary conditions. While stable radiation products can be studied after irradiation at room temperature, the initial and usually thermally very unstable oxidation and reduction species can only be trapped by irradiating *in situ* at low temperature.

As an example, we will focus on the disaccharide sucrose (table sugar) for which we have made substantial progress in recent years. We determined highly accurate *g* tensors and proton hyperfine tensors for the dominant radiation-induced radicals and identified, via DFT calculations, all three as species with a broken glycosidic bond and a carbonyl group in a *beta* position. These experimental data should also enable reliable simulation of the complex EPR spectrum – which has been a major obstacle for exploiting sucrose as (emergency) dosimeter.